# The role of ligands in controlling the electronic structure and magnetic properties of $Mn_4$ single-molecule magnets

Tuan N.A., Katayama S.-i., Chi D.H.

School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Nomi, Ishikawa, 923-1292, Japan; Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Viet Nam

Abstract: We present our studies of electronic structure and magnetic properties of $Mn^{4+}Mn_3^{3+}$ single-molecule magnets (SMM), i.e, $[Mn^{4+}Mn_3^{3+}O_3Cl_4(OAc)_3(py)_3]$ (py = pyridine) and $[Mn^{4+}Mn_3^{3+}O_3Cl(OAc)_3(dbm)_3]$ (dbmH = dibenzoyl-methane) molecules by using a first-principles all-electron relativistic method within spin-polarized density functional theory. To investigate the possibility of ligands controlling the electronic structure and magnetic properties, we designed and calculated the geometric and electronic structures of twelve other $Mn^{4+}Mn_3^{n+}$ (n = 2, 3, 4) molecules with different peripheral-ligand configurations. The electronic structure of $Mn^{n+}$ ions, and the interatomic distances, electronic structure and magnetic properties of $Mn^{4+}Mn_3^{n+}$ molecules display an interesting variation with n. ?? 2008 Elsevier B.V. All rights reserved.

Author Keywords: First-principles calculation; Mn clusters; Molecular design; Nano-piezomagnets; Single-molecule magnets

Index Keywords: Density functional theory; Electronic properties; Electronic structure; Ligands; Magnetic materials; Magnetic properties; Magnets; Manganese; Manganese alloys; Methane; Molecules; Solid state physics; Structural properties; First-principles calculation; Mn clusters; Molecular design; Nano-piezomagnets; Single-molecule magnets; Manganese compounds

Year: 2008

Source title: Computational Materials Science

Volume: 44

Issue: 1

Page : 111-116

Link: Scorpus Link

Correspondence Address: Chi, D.H.; School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Nomi, Ishikawa, 923-1292, Japan; email: dam@jaist.ac.jp

ISSN: 9270256

CODEN: CMMSE

DOI: 10.1016/j.commatsci.2008.01.060

Language of Original Document: English

Abbreviated Source Title: Computational Materials Science

Document Type: Article

Source: Scopus

Authors with affiliations:

1. Tuan, N.A., School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Nomi, Ishikawa, 923-1292, Japan, Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Viet Nam
2. Katayama, S.-i., School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Nomi, Ishikawa, 923-1292, Japan
3. Chi, D.H., School of Materials Science, Japan Advanced Institute of Science and Technology, 1-1, Asahidai, Nomi, Ishikawa, 923-1292, Japan, Faculty of Physics, Hanoi University of Science, 334 Nguyen Trai, Thanh Xuan, Hanoi, Viet Nam

References:

1. Wang, S., Tsai, H.-L., Libby, E., Folting, K., Streib, W.E., Hendrickson, D.N., Christou, G., (1996) Inorg. Chem., 35, p. 7578
2. Hammer, B., (1999) Phys. Rev. B, 59, p. 7413
3. Wernsdorfer, W., Aliaga-Alcalde, N., Christou, G., (2003) Science, 302, p. 1015
4. Hendrickson, D.N., Christou, G., Schmitt, E.A., Libby, E., Bashkin, J.S., Wang, S., Tsai, H.-L., Streib, W.E., (1992) J. Am. Chem. Soc., 114, p. 2455
5. Aubin, S.M.J., Dilley, N.R., Pardi, L., Krzystek, J., Wemple, M.W., Brunel, L.-C., Maple, M.B., Hendrickson, D.N., (1998) J. Am. Chem. Soc., 120, p. 4991
6. Andres, H., Basler, R., G?del, H.-U., Arom??, G., Christou, G., B?ttner, H., Ruffl??, B., (2000) J. Am. Chem. Soc., 122, p. 12469
7. Pederson, M.R., Khanna, S.N., (1999) Phys. Rev. B, 59, pp. R693
8. Hill, S., Edwards, R.S., Aliaga-Alcalde, N., Christou, G., (2003) Science, 302, p. 1015
9. Park, K., Pederson, M.R., Richardson, S.L., Aliaga-Alcalde, N., Christou, G., (2003) Phys. Rev. B, 68, pp. R020405
10. Delley, B., (1990) J. Chem. Phys., 92, p. 508
11. Delley, B., (1998) Int. J. Quantum Chem., 69, p. 423
12. Delley, B., (2000) J. Chem. Phys., 113, p. 7756
13. Delley, B., (2002) Phys. Rev. B, 65, p. 085403
14. Kessi, A., Delley, B., (1998) Int. J. Quantum Chem., 68, p. 135
15. Hehre, W.J., Radom, L., Schlyer, P.v.R., Pople, J.A., (1986) Ab Initio Molecular Orbital Theory, , Wiley, New York
16. Hammer, B., Hansen, L.B., N??rskov, J.K., (1999) Phys. Rev. B, 59, p. 7413
17. Matveev, A., Staufer, M., Mayer, M., R??sch, N., (1999) Int. J. Quantum Chem., 75, p. 863
18. Han, M.J., Ozaki, T., Yu, J., (2004) Phys. Rev. B, 70, p. 184421

Download Full Text: 0439.pdf